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EXCITATION CONDITIONS IN THE UPPER ATMOSPHERE AS DETERMINED FROM A STUDY OF ATOMIC EMISSION LINES IN THE AURORAL SPECTRUM[1]

BY WILLIAM PETRIE[2]

Abstract

Vegard's identifications of a number of lines appearing in the auroral spectrum are discussed. The conclusion is reached that a good many of these lines may be attributed to the oxygen atom in several stages of ionization. It is shown how measured line intensities and theoretical line strengths are combined to give the excitation temperature of the auroral region. Preliminary results indicate that this temperature is in the range 3000° to 6000° K. The meaning of this result is discussed briefly.

Introduction

It is well known that the auroral spectrum is dominated by nitrogen bands, and lines arising from the lower levels of the oxygen atom. The extensive observations by Vegard and Tönsberg (12) suggest that a number of the weaker spectral features may be attributed to oxygen and nitrogen atoms in several different stages of ionization. It is important that intensity measures of these features may be obtained, since such data will give information on the excitation conditions of the upper atmosphere. In this paper, Vegard's identification of certain of the weaker lines is discussed, and it is shown how measured intensities and theoretical strengths for these same lines may be used to compute the temperature of the auroral region.

Discussion of Vegard's Data

In order to decide which oxygen and nitrogen lines are likely to appear in the auroral spectrum, it is necessary to study the energy levels of these atoms, and to consider the transition probabilities between various levels.

(*a*) OI

The ground levels of the neutral oxygen atom are ^3P, ^1D, ^1S, the latter two being metastable levels. Transitions between the $^1D - {}^3P$ levels produce the red auroral lines at λλ 6364, 6302. Transitions between the levels $^1S - {}^1D$ produce the green auroral line at λ 5577. A third transition, $^1S - {}^3P$ gives a line at λ 2972, which has not been observed in the auroral spectrum. Consider the 'future' of atoms excited to the ^1S level. Radiative transitions may take place to the levels ^1D and ^3P, forming the lines λλ 5577, 2972. Since the

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transition probabilities to the levels ^1D and ^3P are in the ratio 2.0 : 0.18, we would expect the latter line to be formed with appreciable intensity. The values of the transition probabilities have been calculated by Bowen (2). However, a number of the atoms in the ^1S level will be collisionally de-excited to the ^1D and ^3P levels; these are radiationless transitions. The intensity of the line λ 2972 will depend upon the ratio between the two types of transitions.

The theory of collisional excitation and de-excitation has been used by Menzel and colleagues (8), to compute temperatures in the atmospheres of a number of planetary nebulae. Consider two energy levels A and B. Let N_A = the number of atoms per cubic centimetre in level A, and let N_e = the number of free electrons per cubic centimetre. Then the number of collisional excitations by electrons from A to B per second is (4):

$$N_{AB} = N_A N_e \int_{v_0}^{\infty} \Omega_{AB}\, v\, f(v)\, dv\ . \tag{1}$$

Ω_{AB} = the cross-sectional area for collisional excitation by electrons from levels A to B. $f(v)$ = the fraction of the electrons with velocities between v and $(v + dv)$. If we assume that a Maxwellian velocity distribution holds for the free electrons, then,

$$f(v)\, dv = 4\pi \left(\frac{m}{2\pi k\, T_e}\right)^{\frac{3}{2}} v^2 e^{-\frac{1}{2}mv^2/kT_e}\, dv\ . \tag{2}$$

T_e is called the electron temperature, that is, the temperature controlling the velocity distribution among the free electrons. v_0 is the smallest electron velocity capable of exciting the atom from level A to B, and is defined by

$$\tfrac{1}{2}\, mv_0^2 = \chi_{AB}\ . \tag{3}$$

χ_{AB} = the difference in excitation potential between the levels A and B. Carrying out the integration and substituting the values of the constants, we find for inelastic collisions,

$$N_{AB} = 8.54 \times 10^{-6}\, \frac{N_A\, N_e}{T_e^{\frac{1}{2}}}\, \frac{\Omega_{AB}}{\tilde{\omega}_A}\, e^{-\chi_{AB}/kT_e}\ . \tag{4}$$

$\tilde{\omega}_A$ = the statistical weight of level A. For superelastic impacts, the number of collisional de-excitations per second from levels B to A is,

$$N_{BA} = 8.54 \times 10^{-6}\, \frac{N_B\, N_e}{T_e^{\frac{1}{2}}}\, \frac{\Omega_{AB}}{\tilde{\omega}_B}\ . \tag{5}$$

$\tilde{\omega}_B$ = the statistical weight of level B. The exponential does not appear since electrons of any velocity may bring about de-excitation.

We will now use Equation (5) to calculate the number of collisional de-excitations from the levels ^1S to ^3P. Collisional cross-sections for the OI atom have been calculated by Yamanouchi *et al.* (14). Their value for

$\Omega_{SP} = 2.5$. The value of $\tilde{\omega} = (2J + 1) = 1$ for the $^1S_0$ level. Martyn and Pulley (7) give the electron density in the auroral region as 10^5 per cm.^{3} The work of the same authors indicates that the electron temperature in the auroral region is 1200° K. Substituting these values in Equation (5) we have

$$N_{SP} = 8.54 \times 10^{-6} \frac{N_e \times 10^5}{(1200)^{\frac{1}{2}}} \frac{2.5}{1} = 0.06\, N_e .$$

This result indicates that 6% of the atoms in the ^1S level are collisionally de-excited to the ^3P levels. A similar calculation shows that about the same percentage are collisionally de-excited to the ^1D level. Hence the greatest number of the atoms in the ^1S level experience radiative transitions to the ^1D and ^3P levels, and the line λ 2972 should appear with appreciable intensity. It is likely that this radiation is absorbed by the ozone layer, which would account for its non-appearance. It is intended to carry out a laboratory investigation of this point at the University of Saskatchewan.

In addition to the red and green auroral lines, Vegard and Tönsberg (12) list several others as being due to OI. Four of these appear to arise from the following transitions.

$$2p^3 5s(^5S^0) - 2p^3 3p(^5P) \text{ giving } \lambda\, 6453.7$$

$$2p^3 4p(^5P) - 2p^3 3s(^5S^0) \text{ giving } \lambda\, 3947.3$$

$$2p^3 4p(^3P) - 2p^3 3s(^3S^0) \text{ giving } \lambda\, 4368.3$$

$$2p^3 3s(^3P^0) - 2p^3 3p(^3P) \text{ giving } \lambda\, 3954.6$$

The identifications are doubtful with the exception of the line λ 4368.3. The lines λλ 6453.7, 3947.3 are moderately strong, but fall very close to nitrogen bands of the first and second positive group. These will be denoted by $1P.G.$ and $2P.G.$ The line λ 3954.6 has a small theoretical strength, and is listed as a weak feature in the M.I.T. wave-length tables. The identification of the line λ 4368.3 is probably correct; it is the strongest line in the multiplet formed by the transitions $^3P - {}^3S$, and is listed as a high intensity line in the M.I.T. tables.

There are strong lines arising from other levels of the OI atom. Since these lines have not been recorded in the auroral spectrum, their absence must be satisfactorily explained if the identification of λ 4368.3 is correct. An examination of these levels shows that the lines arising from them are either in the region of nitrogen bands, or else appear in the near infrared beyond the present recorded auroral spectrum. The detection in the auroral spectrum of the line λ 8446.4 from the transition $2p^3 3p(^3P) - 2p^3 3s(^3S^0)$, would greatly strengthen the identification of the other OI permitted lines. This feature should be searched for carefully, since it has a large theoretical strength,

appears as a strong line in the M.I.T. tables, probably falls in a clear region between members of the 1*P.G.* nitrogen bands, and would not be strongly absorbed by the atmosphere below the auroral region. The transitions producing the OI lines discussed here are shown in Fig. 1.

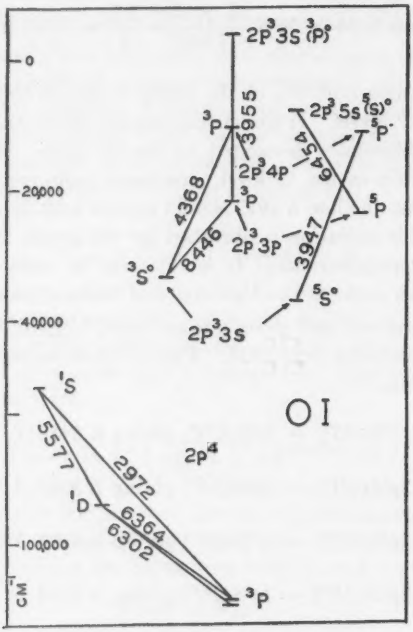

FIG. 1. *Partial energy level diagram of OI.*

(*b*) OII

The ground configuration of the OII atom is $2p^3$, giving the terms ^4S, ^2D, ^2P, the latter two being metastable. The transition $^2D - {}^4S$ gives a line at λ 3728.9, which is observed in the auroral spectrum. Lines from the transition $^2P - {}^2D$ would probably be recorded, but they fall in the region of the 1 *P.G.* nitrogen bands. Vegard lists 25 lines as due to the OII atom, and 14 of these have been assigned to definite energy levels. Table I lists these lines and the transitions from which they arise. The words first, second, and third mean that the line in question is the strongest, second strongest, etc., in the multiplet to which it belongs.

The evidence generally favours Vegard's identifications. Most of these lines have large theoretical strengths, and are listed as strong lines in the M.I.T. tables. The identification of the lines λλ 3954.4 and 3982.7 is in doubt, since these features have small theoretical strengths, and are listed as weak lines in the M.I.T. tables. Strong lines from other levels fall in the

region of nitrogen bands, and hence do not appear. We must explain the absence of the line λ 4943.0 from the transition $2p^23d(^2D) - 2p^23p(^2P^0)$. This line has a large theoretical strength and appears to be in a region free from nitrogen bands.

TABLE I

Transition	Wave-length, Å	Remarks
$2p^23p(^4P^0) - 2p^23s(^4P)$	4319.6	Second. Strongest in region 2*PG* bands
$2p^23p(^2P^0) - 2p^23s(^2P)$	3954.4	Second. Strongest in region Vegard–Kaplan bands
$2p^23p(^2P^0) - 2p^23s(^2P)$	3982.7	Third
$2p^23p(^2D^0) - 2p^23s(^2P)$	4414.9	First
$2p^23p(^2D^0) - 2p^23s(^2P)$	4417.0	Second
$2p^23p(^2D^0) - 2p^23s(^2P)$	4452.4	Third
$2p^23d(^4F) - 2p^23p(^4D^0)$	4075.9	First
$2p^23d(^4F) - 2p^23p(^4D^0)$	4072.2	Second
$2p^23d(^4D) - 2p^23p(^4D^0)$	3857.2	Second. Strongest in region of Negative Group nitrogen bands
$2p^23d(^4D) - 2p^23p(^4P^0)$	4119.2	First
$2p^23d(^2G) - 2p^23p(^2F^0)$	4185.5	Second. Strongest in region of Negative Group nitrogen bands
$2p^24f(^4F^0) - 2p^23d(^4F)$	4048.2	Second. Strongest in region of 2*PG* bands
$2p^24f(^4D^0) - 2p^23d(^4P)$	4303.8	First
$2p^24f(^4D^0) - 2p^23d(^4P)$	4294.7	Second

(*c*) OIII

The ground configuration of the OIII atom is $2p^2$, giving the terms $^3P, ^1D, ^1S$, the latter two being metastable. The transition $^1D - ^3P$ gives two lines at λλ 4959.0, 5006.8; the latter is listed by Vegard as appearing in the auroral spectrum. The ratio of the transition probabilities of these lines is 0.006 : 0.018, which probably explains the absence of the former line. The line at λ 4363.2 from the transition $^1S - ^1D$ is listed as appearing in the auroral spectrum with considerable intensity. Lines arising from transitions between the lower permitted levels either fall in the region of nitrogen bands, or are beyond the recorded spectral region, with the exception of λ 3962.7 from the transition $2p3p(^1S) - 2p3s(^1P^0)$. This line is given in Vegard's list.

(*d*) NI

The ground configuration of NI is $2p^3$, giving the terms $^4S, ^2D, ^2P$. The transitions $^2D - ^4S$ give a pair of lines with wave-lengths λλ 5198.5 and 5200.7. These lines should be looked for carefully; they do not appear in

Vegard's list. The transition $^2P - {}^4S$ gives a line at λ 3466.4 which is included in Vegard's list. Vegard attributes six additional lines to the NI atom, and three of these appear to arise from the following transitions—

$$2p^24p(^2S^0) - 2p^23s(^2P) \text{ giving } \lambda\, 4935.0$$

$$2p^24p(^2S^0) - 2p^23s(^2P) \text{ giving } \lambda\, 4914.9$$

$$2p^24p(^4P^0) - 2p^23s(^4P) \text{ giving } \lambda\, 4223.0$$

These identifications are in doubt, since all three have small theoretical strengths, and only the first appears as a reasonably strong line in the M.I.T. tables. The line at λ 5560.4 from the transition $2p^25d(^4F) - 2p^23p(^4D^0)$ should be searched for carefully, since it has a large theoretical strength and is listed as an intense line in the M.I.T. tables.

(*e*) NII

The ground configuration of the NII atom is $2p^2$, giving the terms ^3P, ^1D, ^1S. The transitions $^1D - {}^3P$ give lines with wave-lengths λλ 6548.1 and 6583.6. The line at λ6548.1 is listed by Vegard, but the other does not appear. This second line should be searched for carefully since it has the greater transition probability of the pair. It may be obscured by a member of the 1 *P.G.* nitrogen band system. The transition $^1S - {}^1D$ gives a line at λ5754.8, which appears in Vegard's list. A number of additional lines are attributed to NII. One of these, at λ 5679.6, appears to arise from the transition $2p3p(^3D) - 2p3s(^3P^0)$. The identification is probably correct, since this line has a large theoretical strength and appears as an intense line in the M.I.T. tables.

(*f*) NIII

The lower forbidden transitions of the NIII atom are not in the observable region of the spectrum. Two lines listed by Vegard appear to arise from the following transitions $2s2p3p(^4D) - 2s2p3s(^4P^0)$ giving λ 4510.7, $2s2p3p(^4S) - 2s2p3s(^4P^0)$ giving λ 3772.2.

In summary, we may say that the evidence generally favours Vegard's identification as regards the atomic oxygen lines. The case for the appearance of atomic nitrogen lines is not nearly so strong. It is suggested that useful information may be obtained by studying the relative intensities of certain oxygen and nitrogen lines appearing in a discharge through air at various pressures. Such an investigation is being undertaken at the University of Saskatchewan.

Assuming that Vegard's identifications are correct in certain cases, the question arises as to the mechanism of excitation which is operating. A good deal has been written on this subject, since it was necessary to explain the appearance of the forbidden oxygen lines from the ground levels of the atom,

and the absence of all permitted lines from higher levels. Kaplan (6) has suggested that oxygen atoms are excited to the lower metastable levels through collisions with nitrogen molecules in metastable levels. Since Kaplan has observed the auroral green line in a discharge produced mainly by nitrogen molecules in metastable levels, his argument is fairly conclusive. Chapman (3) has suggested that the nitrogen molecules are excited by the energy available from the recombination of oxygen atoms. However, if atomic oxygen lines arising from permitted levels are present, a more general mechanism of excitation must be operating. It is suggested that the most probable mechanism is excitation by electron collision. It is well known that oxygen and nitrogen atoms in both the neutral and ionized forms present large cross-sectional areas for collisional excitation by electrons. Regardless of the method of excitation, the relative populations of a number of energy levels will give information on excitation conditions.

Line Intensities and Line Strengths

The strength of a line is defined as the sum of the absolute squares of the matrix elements of electric moment joining the sets of states in question. On the other hand, the intensity of a line is proportional to the number of atoms in any one of the states of its initial level, the fourth power of its frequency, and its strength. A quantitative expression for the intensity of a spectral line is given by Equation (6)

$$I = \frac{64\pi^4\nu^4}{3c^3} N_0 \frac{\tilde{\omega}}{\tilde{\omega}_0} e^{-\chi_n/kT} s \quad , \tag{6}$$

where ν = the frequency of the line,
N_0 = the number of atoms in the ground level for a particular stage of ionization of the element in question,
$\tilde{\omega}$ = the statistical weight of the level from which the line originates,
$\tilde{\omega}_0$ = the statistical weight of the ground level,
χ_n = the excitation potential of the upper energy level involved in the production of the line,
T = the excitation temperature of the emitting volume,
s = the theoretical line strength.

The strength of a line in terms of the strength of the multiplet to which the line belongs may be obtained from the tables computed by Russell (11). That is, we obtain the quantity $\frac{s}{\Sigma s}$, where s is the line strength and Σs the multiplet strength. Relative multiplet strengths in terms of a quantity σ^2 have been calculated by Goldberg (5). σ is a function of the total and orbital quantum numbers, nl and $n'l'$ of the jumping electron, and is given by

$$\sigma = \frac{e}{\sqrt{4l^2 - 1}} \int_0^\infty r . R(n, l) R(n', l') \, dr \quad , \tag{7}$$

where e is the charge on the electron in electrostatic units, and $R(n, l)$ and $R(n', l')$ are the normalized radial eigenfunctions of the jumping electron. The quantity σ is a constant for all the multiplets arising from a transition between two electron configurations. Multiplet strengths in terms of σ^2 are denoted by S. Menzel and Goldberg (9) have computed factors which reduce the relative multiplet strengths to absolute values. We denote these factors by a. The strength of a line is now the product of the three quantities, $\frac{s}{\Sigma s} Sa$, since Σs and S cancel each other.

It should be pointed out that the calculations for both line and multiplet strengths are accurate only if Russell–Saunders coupling holds. The sum rule provides a check on the accuracy of this type of coupling in any given case. The rule states that the sum of the strengths of all the lines of a multiplet which arise from a common initial level is proportional to the weight $(2J + 1)$ of the initial level. This rule has been applied to the multiplets in which we are interested, and Russell–Saunders coupling appears to hold quite accurately.

Excitation Conditions in the Auroral Region

We have stated that a number of auroral lines can be attributed with a good deal of certainty to the oxygen atom. For certain of these lines Vegard and Tönsberg (12) have published measured intensities. It will now be shown how these intensities are combined with values of the theoretical strengths to determine the excitation temperature of the emitting volume. From Equation (7) the relative intensity of two spectral lines is given by

$$\frac{I_1}{I_2} = \left(\frac{\nu_1}{\nu_2}\right)^4 \frac{\tilde{\omega}_1}{\tilde{\omega}_2} e^{-(\chi_{n_1} - \chi_{n_2})/kT} \frac{S_1}{S_2}. \tag{8}$$

Strictly speaking, we should use different temperatures T_1 and T_2 in the equation, to allow for a likely non-Boltzmann distribution of atoms in the various energy levels. However, since we have insufficient data on intensity measures to determine what type of distribution exists, we assume that T will be the same for the various energy levels. Using the intensity values given by Vegard, and the line strengths obtained as we have indicated, and substituting both in Equation (8) it is found that T varies from 3000° K to 6000° K. This result is from four OII lines. These temperatures cannot be considered accurate owing to the limited intensity data available, but the method will give useful information on excitation conditions in the auroral region, when more measured line intensities are obtained. The same calculations applied to energy levels covering a considerable range in excitation potential will give the distribution of atoms in these levels, and hence information on the excitation temperature.

It is perhaps misleading to use the word temperature in this case. If we consider an atmosphere in thermal equilibrium, all methods of computing the temperature give the same results. This condition does not apply to the

earth's upper atmosphere, and the temperature will vary with the method of computation. From the intensity distribution in a number of nitrogen bands, Vegard has obtained a temperature of around 300° K. This means that the particles exciting the nitrogen molecules have a velocity distribution characteristic of 300° K. On the other hand, as indicated above, the intensities of a number of OII lines indicate that the exciting particles have a velocity distribution characteristic of much higher temperatures, in the range 3000° K. to 6000° K. These differences indicate that the earth's atmosphere is far from a condition of thermal equilibrium. Calculations applied to the intensities of OIII lines would undoubtedly give a still different value. The meaning of the different types of temperature used in the field of astrophysics has been given by Petrie (10).

Other investigations have indicated that the temperature obtained depends upon the method used. From a study of the luminosities of meteors as a function of height, Whipple (13) has found that temperatures increase considerably with height. Martyn and Pulley (7) have studied collisional frequencies between electrons and molecules at the 250 km. level, and find a temperature of 1200° K. From measurements of the width of the auroral green line, Babcock (1) estimates the temperature to be 900°. All this evidence from a number of investigations leaves little doubt as to the reality of the high temperature conditions. We must remember, however, that temperature can have different meanings when dealing with an atmosphere not in thermal equilibrium.

In a later communication, the author will indicate a different method of obtaining temperatures from the relative intensities of atomic lines.

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